Report on Workshop on Modeling and Simulation: Practical Engineering Applications

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1 Overview of the Field of Modeling and Simulation

Computational Science has been called a third branch of science, along with theory and experiment. In truth, it is part of theory and part of experiment, but it is different from either. Many theoretical problems can only be solved using a high performance computer. Modeling and simulation, the major component of computational science, is much more than simply elaborating pure theory. It is a critical tool used to analyze important and varied phenomena such as fluid flow and transport, chemical processing, air pollution, water contamination, nano material design, information, computational chemistry, and phase interfaces. In September 2011, a workshop on Modelling and Simulation was held at the Banff International Research Station (BIRS) in Banff, Alberta. The major focus was the presentation of theoretical modelling and simulation work by researchers and software developers from around the world. It also highlighted activities in the high performance computing area.

2 Recent Developments and Open Problems of Modeling and Simulation

Since 2011, the rapid development of computer power and sophisticated computational techniques has resulted in the application of high performance computing to modelling and simulation with unprecedented accuracy. Their scope has also impacted a wide range of important science and engineering challenges. These challenges are comprehensive emerging issues requiring a thorough understanding of the underlining principles of physics, chemistry, mathematical modelling, numerical solution techniques and computing infrastructure. Their understanding will have profound implications and applications in mathematics, science, engineering, medicine and industry. Rapid economic developments and social issues have significantly increased research in modelling and simulation in these areas. For example, the need to study and understand the complex physical and chemical processes occurring in and around the earth, such as groundwater contamination, oil and gas reservoir production, discovering new oil reserves, ocean hydrodynamics, CO2 storage and sequestration, and air quality control, is all vital to our living environment, economic development, natural resource management and national security. The study of these problems through laboratory experiments, modelling theories and simulation techniques requires interdisciplinary collaborations between engineers, mathematicians, computational scientists and researchers working in industry, government laboratories and academy. Bringing together these experts for a unified focused effort will advance predicting, understanding and optimizing many complex phenomena. The goal of this two-day BIRS workshop on September 1-3, 2017 was to hold lectures that emphasize the rapid development of modelling and simulation theories and their practical engineering applications [1, 2, 3].

3 Workshop Presentation Highlights

The workshop themes include: (A) Mathematics of Multiphase Fluid Flow and Transport; (B) High-Quality Discretization of Flow and Transport; (C) Computational Modeling of Multiscale Phenomena; (D) Parallel Computing; (E) Nonlinear Effects on Propagation Properties of Numerical Models; (F) Interfacial Phenomena in Mineral and Material Processing; (G) Spatially Explicit Carbon and Water Cycle Modelling; (H) Air Pollution and Industrial Wastes.

24 presentations in this workshop have dealt with these topics. Speakers have been carefully selected to ensure that a range of modeling and simulation techniques can be explored. This diversity is necessary in order to address various phenomena arising from emerging issues in the energy and environment sectors [4, 5].

Some of the major presentations are summarized as follows:

The presentation given by Dr. Jesse Zhu covered research related to aspects of particle technology from particle formation, characterization, particle flow to many mathematical and practical applications. His fundamental studies included development of fluidization theory and identification of new regimes, the expansion to liquid-solid fluidization, inverse fluidization and untrafine powder fluidization, and the detailed studies on many fluidized bed reactors.

The presentation given by Dr. Jinyu Sheng covered many modeling and simulation problems on physical oceanography, modelling and prediction of extreme marine events, interaction of ocean waves and currents, air-sea interaction, and tidal and storm-induced circulation.

The presentation given by Dr. Liu Zheng covered his research on mathematical, chemical and biomolecular fundamentals of bioprocessing engineering with special interests in protein conformational transition, nanostructured enzyme catalysts, and formulation of natural product with biological functions.

The presentation given by Dr. Frank Cheng covered mathematical problems in corrosion science and engineering of pipelines, including coating failure mode and effect analysis, cathodic protection shielding, high-voltage alternating current interference, CO2 corrosion, microbial corrosion, flow-accelerated corrosion, and under-deposit pitting corrosion.

The presentation given by Dr. Haibo Niu covered his research related to the fate/transport process of contaminants in marine environment, with a focus on oil spills and development of mathematical models to predict the fate/behaviours of oil to support emergency response.

The presentation given by Dr. Johnny Chen covered modeling and simulation issues in electrochemical energy storage and conversion technologies due to decreasing global fossil fuel supplies and increasing environmental concerns. In order to provide sustainable energy infrastructures and resources for future generations, significant improvements to the current state of these technologies is imperative.

The presentation given by Dr. John Chen covered his scientific research on laboratory experiments, mathematical modeling, and the supporting analyses for recovery of oil and gas resources. In particular, his team work has been focused on lab, modeling and simulation studies of fluid flow and transport in unconventional oil and gas reservoirs (heavy oil, oil sands, and tight and shale oil and gas reservoirs). He shared his industrial collaboration experience with the participants.

The presentation given by Dr. Charles Xu covered his modeling approach in development of highly efficient and cost-effective hydrothermal liquefaction (HTL) processes for energy recovery from various solid wastes/residues and development of catalytic processes and novel catalysts for the production ”green” fuels, chemicals from renewable feedstock, and air emissions control.

The presentation given by Dr. Qiao Sun covered her current research activities around building a modeling framework for mechanical systems using wind turbine as an example. The goal is to be able to combine physics based and data driven models to assist machine health condition assessment and failure prediction. A system level model that includes component models based on underlying physical principles can provide the key to a solution with the much needed fault prediction capabilities. In recent years, her focus is to establish an integrated wind turbine system model that can represent the digital copy of an actual system particularly in terms of its health condition.

The presentation given by Dr. Ying Zheng covered her research related to aspects of chemical reaction Engineering, catalyst synthesis and catalytic processes, her recent interests on catalytic process intensification and her fundamental mathematical studies on new material synthesis, catalysis, reaction mechanism and mass/heat transfer in heterogenous catalysis, reactor and process design.

The presentation given by Dr. Hongbo Zeng covered his research interests in colloid and interface science, functional materials and nanotechnology, with a special focus on intermolecular and surface interactions in soft matter (e.g., polymers, biopolymers, biological systems, surfactants, and emulsions) and mathematical and engineering processes, and development of functional materials with engineering/bioengineering/ environmental applications.

The presentation given by Dr. Laurence Yang covered his current interest focused on cyber-physical-social systems (CPSS) design, data analytics on parallel and distributed (cloud) platforms. The booming growth and rapid development in embedded systems, wireless communications, sensing techniques and emerging support for cloud computing and social networks have enabled researchers and practitioners to create a wide variety of Cyber-Physical-Social Systems (CPSS) that reason intelligently, act autonomously, and respond to the users needs in a context and situation-aware manner. It, as a novel emerging paradigm, has gained popularity within the research community and industry due to the fact that it enables deep fusion among humans, computers, and things.

The presentation given by Dr. Dong Liang covered numerical problems in development of conservative high-order characteristics methods for atmospheric aerosol transports; development of efficient Moving-cut HDMR approach for aerosol chemical process; study of energy laws of electromagnetic waves in metamaterials, and development of energy-conserved S-FDTD schemes for computational electromagnetics; development of efficient mass conservative domain decomposition parallel computing methods for environmental computation and for contamination flow in porous media; and development of optimal control approaches for environmental pollution in atmosphere and in groundwater.

The presentation given by Dr. Huaxiong Huang covered numerical solutions for partial differential equations, mathematical models and scientific computing for problems in science and engineering, and modeling real world problems from industry and medicine.

The presentation given by Dr. Jing Chen covered development of regional and global carbon cycle models using these traits as inputs; development of instruments and methods for the ground measurement of these traits; development of a distributed hydrological model using these traits and other inputs; development of canopy radiative transfer models for remote sensing applications; development of biosphere stable isotope models for global carbon cycle research; development of atmospheric inversion and global carbon assimilation systems for estimating the global carbon cycle using atmospheric CO2 concentration; and development of a long-term forest carbon cycle model with consideration of both disturbance and non-disturbance effects.

The presentation given by Dr. Nancy Chen covered her research in modeling the primary, secondary, and tertiary recovery processes; simulating complex recovery process in unconventional heavy oil bitumen and tight shale formations; and optimizing reservoir development strategies to maximize oil recovery or net present values.

The presentation given by Dr. Yaushu Wong covered numerical solutions for partial differential equations, mathematical model and scientific computing for problems in science and engineering, and data sciences and its applications to real world problems.

The presentation given by Dr. Xianguo Li covered his research centred in thermofluid sciences, including fluid flow, heat and mass transfer, thermodynamics, combustion, energy and power systems.

The presentation given by Dr. Gemma Lu covered her current research focused on the interfacial and surface science, biomimetic materials, nanocomposites/nanomaterials/nanotechnology, and microfluidic systems applicable in energy, environmental and biomedical fields such as sustainable energy, oil recovery enhancement, wastewater and tailings treatment, environmental sensing, CO2 capture and utilizations, and soil remediation.

In addition to the regular workshop presentations, there were also considerable time for interactions between participants. The workshop organizers coordinated round-table sessions where questions and answers were shared. Due to the high-level and interdisciplinary nature of the participants invited, those who attended this proposed workshop were exposed to novel ideas and will build new relationships for future collaborations. The workshop presentations, discussion at the round-table sessions and possible future collaborations among the participants will support significant progress of mathematics, science and engineering modelling and simulation.

4 Scientific Progress Made in Modeling and Simulation

The objective of this workshop is to bring together the worlds top active researchers (and their more junior counterparts) who study energy and environmental modeling and simulation to discuss past, recent, and prospective advances in this area. The speakers have summarized important advances from the past two decades and have discussed the current understandings, the state-of-the-art techniques, and the current major challenges. Each session of this workshop has provided a vehicle for participants to learn novel techniques and new advances in this area of work. The content has been academic in nature while addressing the many significant applications for industry [6, 7].

The ultimate goal of the workshop is to expose workshop participants (in particular, junior researchers) to the latest developments in the field of modeling and simulation, while emphasizing the impact of this field on science, engineering, and industry.

The study of the diverse topics presented in the workshop through laboratory experiments, mathematical theory, and computational techniques requires interdisciplinary collaboration between engineers, mathematicians, computational scientists, and researchers working in industry, government laboratories, and academy. The collaborative work of researchers in this workshop will create meaningful progress in predicting, understanding, and optimizing many complex phenomena. The rational for this two-day BIRS workshop is to hold lectures that pull together the major ideas and recent research results, chart future directions, and address newly emerging issues for energy and environment modeling and simulation. It is anticipated that the participants have left the workshop knowing the future research directions and the needed potential applications.

5 Outcome of the Workshop

The Banff International Research Station is a beautiful location for learning and building relationships. Its common areas have supported our goals to have researchers engaged in discussion throughout the workshop event. We have brought researchers from around the world to share their perspectives, test ideas, and create new connections both intellectually and socially while exploring the latest developments in modeling and simulation. This workshop has promoted, enhanced, and stimulated cross-continental research interactions and collaborations in mathematical sciences and will shape changes in the research work completed with modeling and simulation.

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